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EFFECTS OF QUANTUM CONFINEMENT ENERGY ON THE TRANSMITTANCE OF CADMIUM TELLURIDE (CdTe) WITHIN THE NEAR INFRARED REGION (700-2500NM)[†]

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This study investigates how the energy of quantum confinement affects the transmittance of cadmium telluride, because of the importance of this substance, as it crystallizes in the form of cubes as thin films that are used in solar cells and liquid crystal imaging devices, as well as in infrared optics [1]. The MATLAB computer program version (2012a) was used, which is based on the characteristic matrix theory and Brus model, in addition to the quantum confinement energy equation. We found that the transmittance value of the nano CdTe thin film at normal incidence reaches 96.4% at a quantum confinement energy E_{co} = 2.7eV and at a particle size P_S =2.6nm, while the value reaches 73.6% at a quantum confinement energy E_{co} = 0.01eV and at a particle size of P_S=50nm.
Keywords: *Transmittance; Energy gap; Quantum confinement Energy; Brus model; The characteristic matrix*
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I. INTRODUCTION

Reducing the size of semi-conducting materials to the nano-scale leads to a significant change in their physical properties, so they acquire unique properties that differ from those found in bulk materials [2]. In addition, the mechanical properties are considered at the top of the list of properties benefiting from the small size of the nanoparticles, with the presence of large numbers of atoms of the material on their outer surfaces. The hardness values of these materials will also increase, by reducing the dimensions of the particles of the material. And controlling the arrangement of its atoms [3]. This difference in material properties is due to the increase in surface area compared to volume, and to the of quantization of the energy levels of electrons within a specific dimension. This is known as quantum confinement [4]. Quantum confinement occurs when the particle dimensions of a material are equal to or smaller than the Bohr radius of an electron or hole, and quantum confinement is one of the direct effects of reducing the size of a material to the nanoscale as the energy levels of matter become discrete, its effect is shown by the change in the density of states and the energy gap of the material, thus the optical, electronic and electrical properties of materials become confinement scale dependent [5,6]. Quantum confinement can be in one dimension, that is, electrons or holes are allowed to spread in only one dimension, and their movement is restricted in the other two dimensions, and it is known as quantum wires. And it can be two-dimensional, that is, it allows electrons or holes to spread in two dimensions, and their movement is restricted in the third dimension, and it is known as a quantum energy well, but in the case of quantum dots, the system is described as zero dimensions [7].

II. THE EFFECT OF PARTICLE SIZE ON QUANTUM CONFINEMENT ENERGY

Quantum confinement energy mainly deals with the trapping of electrons .This energy is observed when there is an increase in the energy gap. It is very important because it determines the emission energy of the quantum dot [8]. Quantum dots can be described as semiconductor nanoparticles in which electrons are bound in all three directions. The process of trapping charge carriers in quantum dots leads to volume quantization, and this has important implications for the absorption and emission spectra that shift to short a wavelength as the size of the quantum dot decreases, this means that large quantum dots produce red a light while small quantum dots produce blue light thus the energy gap is tunable by changing the size of the quantum dots (QDs) based on the quantum confinement effect [9]. The equation for the quantum confinement energy for the ground state of quantum dots is given [10]:

$$E_{con} = \frac{\hbar^2\pi^2}{2r_{ps}^2}\ [\frac{1}{m_e^*} + \frac{1}{m_h^*}], \tag{1}$$

where r_{ps} is the radius of a spherical quantum dot, and m_e, m_h are the effective mass of the electron and hole.

By using the Brus model we obtain, the change in the energy gap with the change in particle size due to the effect of quantum confinement. It is an important theoretical model that considers both the effective masses' values of an electron and a hole, the quantum dot energy gap variation value (ΔE_g) is given according to this model in the following equation [11].

$$\Delta E_g = \frac{\hbar^2\pi^2}{2r_{ps}^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] - \frac{1.786\, e^2}{\varepsilon\, r_{ps}} - \frac{0.124 e^4}{h^2\varepsilon^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right]^{-1}. \tag{2}$$

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And also

$$\Delta E_g = E_g^{nano}(r_{ps}) - E_g^{bulk}.$$

With which equation (2) takes the form [12]:

$$E_g^{nano}(r_{ps}) = E_g^{bulk} + \frac{\hbar^2\pi^2}{2r_{ps}^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right] - \frac{1.786\, e^2}{\varepsilon\, r_{ps}} - \frac{0.124e^4}{h^2\varepsilon^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right]^{-1}. \quad (3)$$

The energy gap is inversely proportional to r_{ps}^2, as shown by the second component on the right-hand side of equation (3), Because the third and final terms are so small in comparison to the second term, they can be overlooked. Then equation (3) becomes.

$$E_g^{nano}(r_{ps}) = E_g^{bulk} + \frac{\hbar^2\pi^2}{2r_{ps}^2}\left[\frac{1}{m_e^*} + \frac{1}{m_h^*}\right]. \quad (4)$$

III. THE CHARACTERISTIC MATRIX

When electromagnetic radiation strikes a single thin film with two dividing borders that has been produced on the substrate material as shown in Fig1. Using the characteristic matrix which connects the optical permittivity of the system for any polarization and for both vertical and oblique incidence [13], the continuous tangential elements of the magnetic and electrical fields entering and leaving the system, and it is provided as the following equation [14].

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} cos\delta & isin\delta/\eta_1 \\ i\eta_1 sin\delta & cos\delta \end{bmatrix}\begin{bmatrix} 1 \\ \eta_{sub} \end{bmatrix}. \quad (5)$$

The matrix's elements, which stand in for the electric and magnetic fields, are represented by the letters (B, C). The membrane's optical permittivity is represented by the number η_1, and the substrate's optical permittivity is represented by the number η_{sub}.

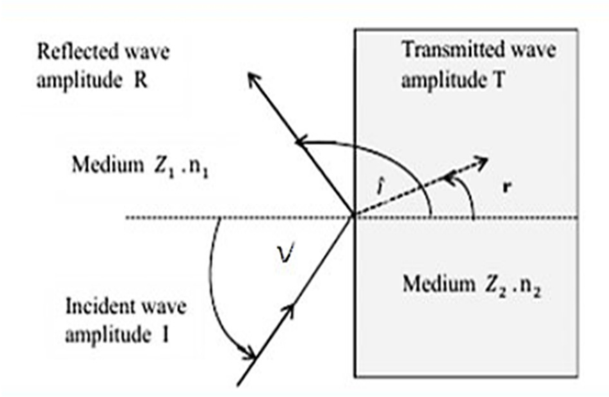

Figure (1) shows the geometry of a plane electromagnetic wave incident on a plane surface [15]

The reflectivity and transmittance value of the electromagnetic beam falling on a surface separating two different media is given by Fresnel's equations [16,15]

$$R = \left(\frac{\eta_\circ - \eta_1}{\eta_\circ + \eta_1}\right)^2, \quad (6)$$

$$T = \frac{4\eta_\circ\eta_1}{(\eta_\circ + \eta_1)^2}, \quad (7)$$

where η_1 and η_o denote the appropriate effective refractive index for the incidence and penetration modes, respectively.

The value of the optical permittivity of the medium in for the vertical incidence of the wave is equal to the real part of the refractive index [17]:

$$\eta = y = n\,\vartheta = n, \quad (8)$$

where n is the real part of the refractive index of the medium, and ϑ is the admittance of free space. Its value may be neglected because it is very small ($2.65\times10^{-3} S$)

Since we use a thin film, the absorbance will be neglected because the thickness of the film is very small, so the reflectivity and transmittance become complementary to each other[4].

IV. ENERGY GAP

A semiconductor atom has a number of electrons in its outer shell, which are distributed into close energy levels as a result of the Pauli exclusion principle, which states that each energy level can accommodate two different electrons in the spin direction [18]. As a result of the convergence of atoms, the individual levels of atoms of matter form a continuous set of energy levels known as energy bands, which represent the entire system when the temperature is zero (T = 0K). In a semiconductor these bands are either fully filled with electrons and known as the valence band, or they are empty known as the conduction band, the valence band is separated from the conduction band by the energy gap, and represents the energy difference between the top of the valence band and the bottom of the valence band delivery [19]. In a direct energy gap semiconductor, the electrons at the top of the valence band have the same momentum (k) as the holes below the conduction band, as shown in the figure (2) where the probability of electron transfer between the two bands is high and the momentum is conserved ($\Delta k = 0$) [20]. The energy gap is closely related to the refractive index, and many attempts have been made to find mathematical equation that link the refractive index with the energy gap, perhaps the most important of which is the equation presented by Ravindra in 1979, which is given in the following equation [21]:

$$n = \alpha + \beta E_g \tag{9}$$

As: ($\alpha = 4.048$) and ($\beta = -0.62$ eV^{-1})this equation is independent of the temperature, and we notice that the value of the refractive index decreases with the increase of the energy gap

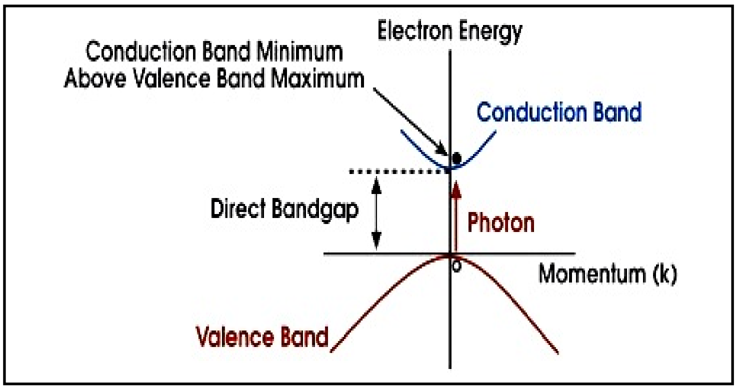

Figure 2. The direct energy gap in the semiconductor material [22]

V. RESULTS AND DISCUSSION

The transmittance change was studied as a function of the change in the quantum confinement energy of cadmium telluride (CdTe) to find out the highest value and the lowest value of the transmittance at which the material reaches as a result of the effect of quantitative confinement on the particle size. We use the MATLAB program version (2012a) which is based on the characteristic matrix and the Brus model in addition to the quantum confinement energy equation.

Fifteen optional incremental values for the radius of the material particles were determined (r_{ps} = 1.3nm to 25nm), through the relationship ($P_S = 2r_{ps}$), we noticed that the material behaves naturally similar to its behavior in the natural state at large size (i.e. bulk material). But with a gradual reduction in size, it was found that there is a wide change in the transmittance of the material, in addition to a wide change in the energy gap, as a result of the effect of quantum confinement on matter.

Table 1. The quantum confinement energy changes with the change of particle size and its effect on the energy gap and transmittance

particle size(nm)	Confinement Energy(eV)	Energy gap(eV)	Transmittance (%) at normal incidence
2.6	2.6587	4.1587	96.3843
2.8	2.2925	3.7925	93.3258
3	1.997	3.497	90.6656
4	1.1233	2.6233	82.7385
5	0.7189	2.2189	79.2631
6	0.4992	1.9992	77.4514
7	0.3668	1.8668	76.3864
8	0.2808	1.7808	75.7063
10	0.1797	1.6797	74.918
12	0.1248	1.6248	74.4949
14	0.0917	1.5917	74.2415
22	0.0371	1.5371	73.8269
30	0.02	1.52	73.6972
40	0.0112	1.5112	73.6313
50	0.0072	1.5072	73.6008

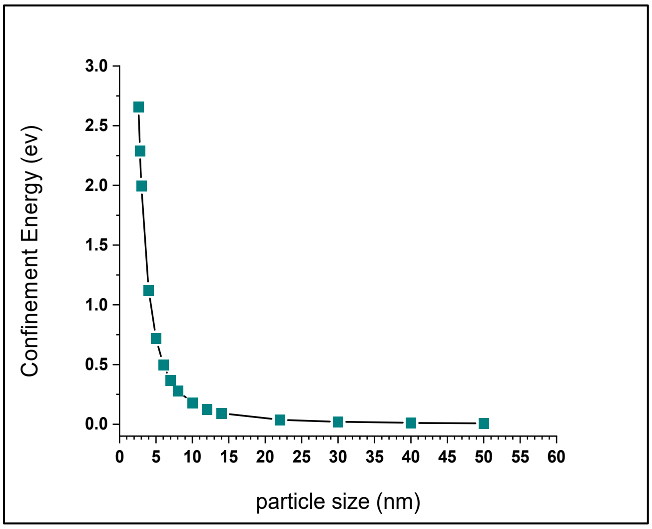

Figure 3. The quantum confinement energy of cadmium telluride (CdTe) as a function of the particle size

We notice from the Figure (3) above that the quantum confinement energy has high values at small nanoscales because the effect of quantum confinement is large when the size of the nanoparticle becomes smaller or equal to the Bohr radius of the natural exciton. while the quantum confinement energy value is low at large nanoscales.

We note from Figure 4&5 that the transmittance at normal incidence increases with the increase in the quantum confinement energy at small nanoscales and begins to decrease when the quantum confinement energy decreases at the large nanoscales. Where it was observed that the transmittance value of the nano CdTe thin film reaches (96.4%) at a quantum confinement energy (E_{co} = 2.7eV) and at a size (P_S = 2.6nm) and at an energy gap (E_g = 4.2eV), while at a size (PS = 50nm) it reaches the transmittance value to (73.6%) at a quantum confinement energy (E_{co}=0.01eV) and at an energy gap (E_g = 1.5eV), This can be explained when the particle size becomes smaller or equal to the Bohr diameter of the natural exciton, the effect of quantum confinement is large, and therefore the energy gap will increase at small sizes, and since the energy gap is inversely proportional to the refractive index as shown in equation (9), its increase It leads to a decrease in the refractive index, a decrease in the refractive index leads to an increase in the transmittance. But when the value of the energy gap decreases when the effect of quantum confinement on the material decreases, then the transmittance value begins to decrease at large sizes.

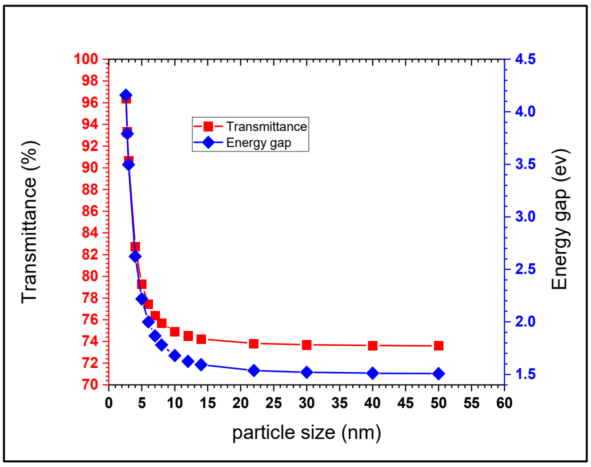

Figure (4) The transmittance at normal incidence and energy gap for cadmium telluride (CdTe)as function of particle size at the nanoscale

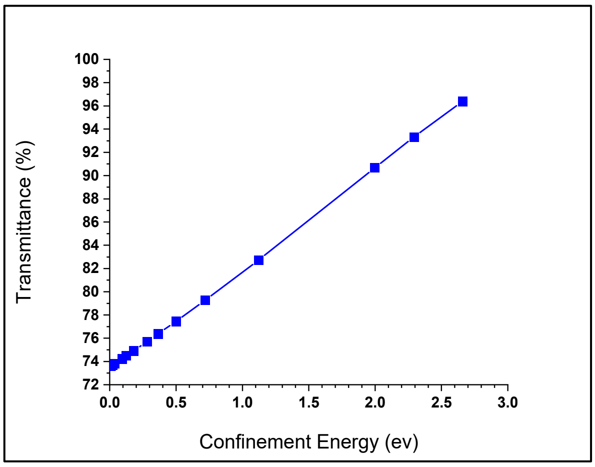

Figure (5) The transmittance of cadmium telluride (CdTe) at normal incidence as a function of the quantum confinement energy

VI. CONCLUSION

It was found that the transmittance at normal incidence of the nano CdTe thin film at the smallest particle size P_S = 2.6nm is as high as 96.4% because the confinement energy is high in the small sizes, while the transmittance at the largest particle size P_S =50nm is low to 73.6% because the quantum confinement energy is low or almost non-existent in the large sizes. The increase in transmittance because the particle size becomes smaller or equal to the normal Bohr diameter of the exciton, the quantum confinement effect increases, and thus the energy gap increases. An increase in the energy gap leads to an increase in the transmittance, while the lower transmittance of the nano CdTe thin film is due to a decrease in the energy gap at these volumes because the quantum confinement effect is very small.

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ВПЛИВ ЕНЕРГІЇ КВАНТОВОГО ОБМЕЖЕННЯ НА ПРОПУСКАННЯ ТЕЛЛУРИДУ КАДМІЮ (CdTe) **В БЛИЖНІЙ ІНФРАЧЕРВОНІЙ ОБЛАСТІ (700-2500 нм)**

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В роботі досліджено, як енергія квантового обмеження впливає на пропускну здатність телуриду кадмію через важливість цієї речовини, оскільки вона кристалізується у формі кубів у вигляді тонких плівок, які використовуються в сонячних елементах і рідкокристалічних пристроях для зображення, а також в інфрачервоній оптиці [1]. Була використана версія комп'ютерної програми MATLAB (2012a), яка базується на теорії характеристичних матриць і моделі Брюса, на додаток до квантового рівняння енергії розміру. Ми виявили, що коефіцієнт пропускання тонкої плівки наноCdTe при нормальному падінні досягає 96,4% при енергії квантового обмеження E_{co} = 2,7 еВ і при розмірі частинок PS = 2,6 нм, тоді як значення досягає 73,6% при енергії квантового обмеження E_{co} = 0,01 еВ і при розмірі частинок P_S=50 нм.

Ключові слова: *пропускна здатність; енергетича щілина; енергія квантового обмеження; модель Бруса; характеристична матриця*